Technical Report Documentation Page

1. REPORT No.
FHWA-CA-TL-7169-76-32

2. GOVERNMENT ACCESSION No.

3. RECIPIENT'S CATALOG No.

4. TITLE AND SUBTITLE
A Consistent Scheme For Estimating Diffusivities To Be Used In Air Quality Models

5. REPORT DATE
June 1976

6. PERFORMING ORGANIZATION

7. AUTHOR(S)
Dr. L.O. Myrup and Andrew J. Ranzieri

8. PERFORMING ORGANIZATION REPORT No.
19701-657169

9. PERFORMING ORGANIZATION NAME AND ADDRESS
Office of Transportation Laboratory
California Department of Transportation
Sacramento, California 95819

10. WORK UNIT No.

11. CONTRACT OR GRANT No.

12. SPONSORING AGENCY NAME AND ADDRESS
California Department of Transportation
Sacramento, California 95807

13. TYPE OF REPORT & PERIOD COVERED
Interim

14. SPONSORING AGENCY CODE

15. SUPPLEMENTARY NOTES
This study was conducted in cooperation with the U.S. Department of Transportation, Federal Highway Administration.

16. ABSTRACT
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17. KEYWORDS
Diffusivity, pollutants, models Pasquill stability classes, land use, mixing length, meteorology, air quality, microscale, mesoscale

18. No. OF PAGES:
73

19. DRI WEBSITE LINK
http://www.dot.ca.gov/hq/research/researchreports/1976-1977/76-32.pdf

20. FILE NAME
76-32.pdf

DIVISION OF STRUCTURES AND ENGINEERING SERVICES

TRANSPORTATION LABORATORY

RESEARCH REPORT

A Consistent Scheme for Estimating Diffusivities To Be Used In Air Quality Models

INTERIM REPORT

FHWA-CA-TL-7160-3-76-32

JUNE 1976

76-32

Prepared in Cooperation with the U.S. Department of Transportation, Federal Highway Administration

Caltrans

CALIFORNIA DEPARTMENT OF TRANSPORTATION

TECHNICAL REPORT STANDARD TITLE PAGE

1. REPORT NO.	2. GOVERNMENT ACCESSION NO.	3. RECIPIENT'S CATALOG NO.
FHWA-CA-TL-7169-76-32		

4. TITLE AND SUBTITLE

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18. DISTRIBUTION STATEMENT

No restrictions. This document is available to the public through the National Technical Information Service, Springfield, VA 22161.

19. SECURITY CLASSIF. (OF THIS REPORT)	20. SECURITY CLASSIF. (OF THIS PAGE)	21. NO. OF PAGES	22. PRICE
Unclassified	Unclassified	73	

DS-TL-1242 (Rev.6/76)

STATE OF CALIFORNIA
DEPARTMENT OF TRANSPORTATION
DIVISION OF STRUCTURES & ENGINEERING SERVICES
OFFICE OF TRANSPORTATION LABORATORY

June 1976

Mr. C. E. Forbes
Chief Engineer

Dear Sir:

I have approved and now submit for your information this interim research report titled:

A CONSISTENT SCHEME FOR ESTIMATING DIFFUSIVITIES
TO BE USED IN AIR QUALITY MODELS

Study made by . . . . Enviro-Chemical Branch

Under the Supervision of . . . . . Earl C. Shirley, P. E.

Principal Investigator . . . . . . Andrew J. Ranzieri, P. E.

Report Prepared by . . . . Dr. L. O. Myrup
and
Andrew J. Ranzieri, P. E.

Very truly yours,

George A. Hill
GEORGE A. HILL
Chief, Office of Transportation Laboratory

Attachment
AJR:bjs

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GLOSSARY OF TERMS

Fp	Flux of "p" in vertical direction
ρ	Air density
Z	Vertical distance
K_p	Vertical diffusivity for quantity p
L	Monin-Obukhov Length
C_p	Specific heat of air at constant pressure
T	Temperature of air
U	Friction velocity
τ	Stress exerted by the ground on the atmosphere
k	Von Karman constant
g	Acceleration of gravity
H	Flux of sensible heat to the atmosphere
Z_o	Aerodynamic roughness parameter
Km	Diffusivity for momentum
$\phi\left(\frac{Z}{L}\right)$	Phi-function for unstable or stable conditions
U	Surface wind speed
Z_w	Height of surface winds measured above average canopy height
ϵ	Dissipation rate (rate at which turbulent kinetic energy is converted to heat)
W*	Convective velocity
Z_i	Height of inversion which caps the convective layer
h_c	Height of canopy or mean height of roughness elements (land use)

ACKNOWLEDGEMENT

This report was written by Dr. Leonard O. Myrup, Associate Professor of Meteorology at the University of California at Davis, consultant to California Department of Transportation and Andrew J. Ranzieri, Senior Materials and Research Engineer.

The authors wish to express their appreciation to Earl C. Shirley and Gerald R. Bemis of the Transportation Laboratory for their review and comments.

The contents of this report reflect the views of the Transportation Laboratory which is responsible for the facts and the accuracy of the data presented herein. The contents do not necessarily reflect the official views or policies of the State of California or the Federal Highway Administration. This report does not constitute a standard, specification, or regulation.

INTRODUCTION

Recent Federal Highway Administration guidelines require any federally aided highway project to evaluate air quality at the project and system level. This analysis is to assure that projects and transportation systems are consistent with regional goals for achieving and maintaining the National Ambient Air Quality Standards.

To comply with federal requirements, the assessment of the impact of transportation systems on the air environment requires the quantitative prediction of pollutant concentrations. These predictions are made on two scales: microscale and mesoscale, or regional area. The microscale region can be defined as the region extending from the point where the pollutants are generated by traffic, downwind to the point where ambient levels are again reached. Figure 1 illustrates this region for a typical roadway. This region is typically 1000 feet or less on either side of the roadway. The mesoscale region is defined as the area throughout which the traffic network is significantly affected by the construction of a new transportation facility. For system planning, this region can be considered to include an entire community or even an air basin. Figure 2 illustrates the build up of pollution for a region. When making predictions using air quality models for either the microscale or mesoscale region, estimates for a pollutant are generally made above some ambient or baseline concentration.

Estimation of concentrations of air pollutants through the use of a regional air quality model requires the study of a large number of variables. Some of these variables, depending on the study region and the model selected, include:

- temporal and spatial distributions of mobile and stationary source emissions,

- wind speed and direction, both at the surface and aloft, as a function of time and space,

- vertical temperature profile as a function of time and space,

- vertical turbulent diffusivity as a function of height, ground location, and time,

- incoming ultraviolet radiation as a function of ground elevation and time,

- temporal and spatial distribution of the initial concentrations of reactive hydrocarbons, oxides of nitrogen, ozone, and carbon monoxide.

One of the major variables is the vertical turbulent diffusivity parameter (or stability parameter) which controls the rate of mass transfer in the vertical direction. This parameter affects such factors as the rate at which plumes rise and their behavior. It also affects the rate at which pollutants are transported and diffused downwind. Figures 3 and 4 illustrate the extreme conditions of stability parameter influence on downwind transport and diffusion of pollutants emitted from a highway on an elevated section (viaduct). Figure 3 characterizes the dispersion of pollutants downwind for a looping plume. Here there is a large degree of thermal turbulence which results in instability (vertical accelerations) near the ground surface causing the looping effect. This would correspond to a daytime condition with clear skies and light winds. Figure 4 characterizes the downwind transport and diffusion of pollutants for a stable atmospheric condition. This generally results in a fanning plume for which the time averaged pollutant concentrations are relatively high within the plume boundaries as compared to those within a looping plume. A fanning plume is generally associated with nighttime conditions of clear skies and light winds. The important point here is to realize that, given the same emission flux and point of release, the atmospheric conditions or the stability parameter will dictate the downwind transport and diffusion.

At present the most widely used methods to estimate atmospheric stability are: (1) Pasquill Stability Categories(1); (2) Turner's(2) approach of classifying stabilities from meteorological measurements of wind speed, cloud cover and ceiling height; (3) measurements of the vertical temperature structure using radar, balloons, or aircraft flights.

The Pasquill and Turner approaches are gross at best. Existing data bases of the vertical temperature profile are extremely limited or nonexistent for purposes of air quality modeling.

Observations and sensitivity analyses of complex boundary layer models indicate strongly that vertical diffusion is a first-order determinant of almost all properties of the air near the surface of the earth. It is mandatory that this process be estimated according to the best available information from practice and theory. Fortunately, this is an area in which great progress has been made in recent years. As a result, it is no longer acceptable to use "diffusion coefficients" as free parameters to be adjusted to cause model output to agree with observations. The diffusivity model described below is consistent with the latest developments in atmospheric boundary layer theory and is supported by observations and numerical calculations. Complete details on the background theory are given by Myrup and Ranzieri(3).

It is the purpose of this report to discuss a method to calculate the vertical turbulent diffusivity, one of the most important atmospheric parameters in air quality models.

CONCLUSIONS

A vertical diffusivity model was developed which takes into consideration (1) land use, (2) evapotranspiration, (3) Turner's Surface Stability Categories, (4) inversion heights, (5) Monin-Obukhov length, (6) surface winds and (7) local stability. The model will allow transportation planners and engineers to further refine the interrelationships between land use, transportation, and air quality and provide information for decision makers.

From the analysis of the model it can be concluded that:

1. Land use significantly affects the vertical diffusivity profile by as much as a factor of ten when considering urban areas vs rural areas.

2. Typical changes in the average canopy height can affect the vertical diffusivity profile by as much as a factor of two for urban areas.

RECOMMENDATIONS

Based on this research the authors recommend the following:

1. This vertical diffusivity model be integrated with conservation of mass air quality models that are used to assess the regional impact of transportation systems on the air environment.

2. Uniform or consistent exposure criteria for locating wind stations be used to develop the data base required for the implementation of this model.

3. The instantaneous measurements of wind speeds, as recorded at airports, should not be used to calculate vertical diffusivity with the model described in this report. This can result in wind data that are not representative of a one hour period and can significantly effect the diffusivities calculated.

4. Wind speeds used in the model should be based on a one hour integrated averaging time.

BACKGROUND

The vertical diffusivity for any quantity p is defined by the following relationship:

$$F_p = -\rho K_p \frac{\partial \bar{p}}{\partial Z} \qquad (1)$$

In this formula F_p is the flux of p in the vertical direction, ρ is the air density, z is the vertical direction and the overbar indicates an averaging process (of the order of 0.5 hour or greater if the averaging is temporal). This definition is based on an analogy with molecular diffusivities. Unfortunately, diffusion in the atmosphere is due to turbulent mixing and the diffusivity defined by equation (1) (often called "eddy diffusivity") is not a constant to be looked up in a handbook but is instead a complex function of the fluid motion and its stratification. Therefore, equation (1) is only a definition and no implication is meant that K_p is a constant. In fact, it should be kept in mind that "eddy diffusivity" has been considered to be a non-physical concept and one which modern experimentalists and theorists largely ignore. However, it is difficult to see how the effects of small-scale turbulence can be included in complex models of other processes, such as general circulation or photochemical air pollution models, in any other way than by the use of the diffusivity concept.

Micrometeorological experience by Businger, et al(4) indicates that diffusivity is a strong function of atmospheric stability, which is specified most basically by the quantity $z/_L$ where L is the Monin-Obukhov length as described in the following equation:

$$L = \frac{-\rho\, C_p\, T\, U_*^3}{k\, g\, H} \qquad (2)$$

Z is the height above the ground surface, C_p is the specific heat capacity of air at constant pressure, T is air temperature in ^oK, U_* is the "friction velocity" as defined in the following equation:

$$U_* = \left(\frac{\tau}{\rho}\right)^{\frac{1}{2}} \tag{3}$$

where τ is the stress exerted by the ground on the atmosphere, k is the von Karman constant with a value of 0.35, g is the acceleration of gravity, and H is the flux of sensible heat to the atmosphere. The quantity $z/_L$ is negative for unstable stratification and positive for stable conditions. The physical interpretation of the Monin-Obukhov length is that this is the approximate height above the surface at which buoyancy effects become comparable with shear effects, which dominate below this height. The physical interpretation of the Monin-Obukhov length under stable conditions (L = positive) is that L equals roughly the height at which vertical turbulence is suppressed. Under very stable conditions L becomes small and resultant downwind air pollutant concentrations are high.

Under unstable conditions, L is negative and has the physical interpretation as being the height at which convectively produced turbulent energy compares with mechanically produced energy. Above a height equal to L, bouyancy driven convection predominates and under these conditions, turbulence is higher, atmospheric diffusion more efficient and downwind pollutant concentrations less. When the absolute value of L approaches infinity $|L| \to \infty$ this is comparable to neutral atmospheric conditions. In summary, L has the following interpretation:

L	Value	Atmospheric Stability Condition
$L \leq -100$ m	Large negative	Unstable
-100 m $\leq L \leq -10$ m	Small negative	Very unstable
$\lvert L \rvert > 10^5$m	∞	Neutral
$L < 10$ m	Small positive	Very stable
$L > 10$ m	Large positive	Stable

Needless to say the Monin-Obukhov length is not a quantity which is routinely measured and available from the local weather office. However, L may be estimated from conventional weather data.

The most common surface stability classification scheme used in air pollution meteorology was originally devised by Pasquill(1) and later modified by Turner(2). Essentially, Pasquill category is a function of the radiation balance of the surface of the earth and the wind speed. Pasquill and Turner surface stabilities are generally categorized in seven classes as follows:

A = extremely unstable
B = unstable
C = slightly unstable
D = neutral
E = slightly stable
F = stable
G = very stable

Stability Class A is generally associated with convective turbulence caused by strong solar heating during daytime conditions with clear skies and light winds. At the other extreme, Stability Class G is associated with a stable atmosphere where turbulence is suppressed. These conditions generally occur during the night and early morning with clear skies and light winds. Detailed directions for calculating Pasquill stability categories with computer programs are given in

Beaton, et al(6). It would be of great practical utility to be able to convert Pasquill categories to values of L. There are problems in doing this, however. When the Pasquill category is calculated for a given region, it applies at all locations that have the same land-use. Unfortunately, land-use almost always presents a checker-board appearance on a regional scale and the microclimate and local stability ($z/_L$) can vary enormously within the region for a given Pasquill category. There are four factors which control local stability. These are:

1. surface roughness,
2. evaporation,
3. anthropogenic generation of heat, and
4. surface physical properties (albedo, heat conductivity and capacity, emissivity, etc.).

Surface roughness is a prime factor because it directly affects the turbulence level near the ground. Local evaporation rates (or evapotranspiration if plants are responsible for the evaporation), are a factor because the energy used in transforming water from the liquid to the vapor state is then unavailable to heat the underlying surface or air. Consequently, local areas of high evaporation are noticeably cooler and generate less thermal turbulence. Heat released from human activities, such as transportation systems, industrial operations or space heating, affects local stability directly through low level heat input. This has the effect of preventing low-level inversions and augmenting thermal turbulence. Surface physical properties affect local stability through their influence on the radiation balance of the surface of the earth. For instance, a high albedo ratio (reflectivity to solar radiation) means that less energy is available to heat the surface and air and, hence, less thermal turbulence will result. The order in which these four factors are listed above is also their order of importance in most land-uses for controlling local stability. The relative importance of anthropogenic heating is most variable. It is possible that in local areas of very heavy energy use, this factor may be comparable in importance to surface roughness. Conversely, in many land uses, human-generated energy is of no importance whatsoever.

Golder[7] has compiled an empirical relationship between Pasquill stability category, calculated in the usual manner, and values of $1/_L$. Golder takes only surface roughness into account. The data he uses are from sites where human energy release would not be present and surface physical properties would be generally the same. Evaporation, however, remains problematical in this analysis. Golder's thesis gives values of $1/_L$ as a function of the Pasquill categories A through G and the aerodynamic roughness parameter z_o (to be discussed below). The agreement between the two approaches to stability parameterization is moderately good. The overall separation between stable and unstable conditions is good and these data clearly show a tendency for $1/_L$ to approach zero for large roughness values. The authors interpretate the scatter in Golder's results as being due to the importance of evaporation in the basic data. It is concluded that, except in local areas of intense energy use, local stability is primarily determined by local roughness and surface stability, as specified by the Pasquill system of categories.

Sutton(8) has shown that the roughness parameter, z_o, is a measure of site roughness characteristics, and may be inferred from measurements of wind shear if these data are available. Plate(5) and Myrup, et al(9) have shown that z_o can be determined from knowledge of the size of typical roughness elements or the land-use of the surrounding terrain. Table 1 below gives values of z_o from Sellers[10] and Myrup et al[9].

TABLE 1

Roughness Heights for Various Surfaces

Type of Surface	Z_o (cm)
Smooth mud flats	0.001
Tarmac	0.002
Dry lake bed	0.003
Smooth desert	0.03
Grass (5-6 cm)	0.75
(4 cm)	0.14
Alfalfa (15.2 cm)	2.72
Grass (60-70 cm)	11.4
Wheat (60 cm)	22
Corn (220 cm)	74
Citrus Orchard	198
Fir forest	283
City land-use	
Light density residential	108
Heavy density residential	370
Office	175
Central Business District	321
Park	127

Table 2 describes the land-use categories in detail for city land use based on data from Myrup(9).

Alternatively Plate(5) has shown that Z_o may be calculated from the simple formula:

$$Z_0 = 0.15\ h_c \tag{4}$$

where h_c is the "canopy height", i.e., the mean height of the surface roughness elements which vary with land use classification. For transportation planners and engineers, equation (4) is the most practical to use for large study areas rather than values of Z_o given in Table 1 which are derived for the Sacramento, California, study region by Myrup(9).

Figures 5 and 6 show the relationship between the roughness parameter, Z_o, Pasquill stability categories and the quantity $1/_L$ (local stability at a height of 1 meter). The figures are based on Golder's data(7) extended to the larger roughness values of the urban environment. Thus, Figures 5 and 6 may be used to convert Pasquill stability categories to values of 1/L on the basis of quantitative information concerning site roughness characteristics, and qualitative estimates of the importance of evaporation. These two factors should dominate local stability under all conditions.

In the winter and summer the effects of anthropogenic heating (urban heat island effect) may, under some circumstances, become the dominant effect. Anthropogenic heating in large urban areas can be caused by:

1. combustion and dissipation of fuel energies from motor vehicles, industrial complexes and domestic heating.

2. blanketing effect at night of pollutant clouds that absorb and re-emit thermal radiation from the city, resulting in large nocturnal temperature excesses.

3. reduced evaporation or plant transpiration in large urban areas.

4. manmade surfaces (concrete, asphalts, etc) have large heat capacities and conductivities.

In general, these arguments suggest strongly that the urban heat island is a result of a complex set of interacting physical processes.

The urban heat island effects are largest in areas with high population and much industry. In cold climates this effect can become more pronounced. Studies made by Atwater(11) and Munn(12) indicate that local urban stability is substantially altered towards neutral stability. However, the researchers found that low level inversions do occur.

Since a reliable quantitative means for taking into account the effects of the urban heat island does not exist at this time, the authors decided to adopt a conservative approach. We recommend the following procedure for all seasons of the year:

1. In rural areas, the Pasquill stability categories should be calculated from available meteorological data. The stability categories can then be converted to values of $1/_L$ using Figures 5 and 6, taking into account land use as described above.

2. In urban areas, a correction factor should be applied to the calculated Pasquill stability category to allow for the urban heat island effect. It is recommended that the calculated Pasquill category be moved one category towards the unstable condition. By this we mean, a calculated F category becomes E, E becomes D, etc. The user of this approach should be aware that this is an interim procedure and more precise means for taking into account the urban heat island may become available in the future.

The exact boundaries of an urban heat island for a given study region are difficult to define. Therefore, the geographical extent of this effect must be selected based on judgment, type of land use, population densities, etc. More research is needed to fully define the area wide extent of the urban heat island.

In Figure 6, the curve for moderate evaporation for F stability was added to the diagram. This was based on a study made by Myrup and Morgan(9) on the numerical simulation of the heat budget for the City of Sacramento, California, for summertime conditions.

These figures specify only a range of values for $1/_L$ for a given Pasquill category and roughness height. This is inherent in the data and we presume due primarily to variations in evaporation from site to site. Therefore, for each stability category, we have indicated the more stable values of $1/_L$ to be associated with high evaporation and the less stable values to low evaporation. Experience in micrometeorology (Sutton(8), and Sellers(10) and Myrup, et al(9) in urban meteorology, indicates that irrigated crops, parks and open water are high evaporation areas. The predominant land-use category in urban areas, light density residential, is a moderate evaporation area. On the other hand, the central business district, industrial, office building and shopping land-use categories are characterized by low evaporation. Table 3 is a summary of the evaporation rates determined by Myrup, et al(9). This table can be used as a guideline to select evaporation rates as a function of land use.

TABLE 2

LAND-USE CATEGORIES

Category	Description
Light-density residential	Single-family unit dwelling (8 family units per acre limit)
Heavy-density residential	Dense apartment area, boarding house type (87 family units per acre limit)
Office buildings	High rise professional office building area
Central Business District	Downtown area, department stores, office buildings and concentrated business activities
Seasonal green	Agricultural areas
Open green	Undeveloped areas with natural annual grass and weed cover
Park	Designated parks, maintained year-round

TABLE 3

Evaporation and Land-use for Sacramento, California, 1971

Land-Use Type	Percent Green Area	Evaporation
Seasonal Green	100	High
Park	93	High
Light-density residential	45	Moderate
Medium-density residential	56	Moderate
Heavy-density residential	43	Moderate
Schools	35	Moderate
Shopping	4	Low
Office	13	Low
Central Business District	7	Low
Industrial	1	Low
Open Green	5	Low

The definition of diffusivity implied by equation (1) may be specialized to any of several quantities. Diffusivities for momentum, heat and water vapor are most commonly measured in micrometeorological investigations and are consequently best known. Diffusivity for momentum is generally regarded as the most important inasmuch as momentum transport is intrinsically involved with the entire phenomenon of turbulence. To the authors knowledge no diffusivities for air pollutants have been directly measured (i.e., simultaneous measurement of both flux and gradient) in a carefully controlled experiment. Therefore, we choose here to select the diffusivity for momentum to use to calculate the vertical flux of any gaseous air pollutant. It might appear that the diffusivity for water vapor might be the most appropriate to use for pollutant transfer inasmuch as both are mass fluxes. However, it is known that water vapor transfer is influenced by buoyancy forces arising out of the fact that water vapor is a lighter gas than dry air. When evaporation rates are large under unstable stratification, water vapor diffusivity is markedly increased over the value for momentum. No pollutant gases reach concentration levels to compare with water vapor, (1 to 2% by mass). However we conclude that molecular weight should not be a factor. Hence, all pollutants should diffuse according to the momentum diffusion theory.

THE DIFFUSIVITY MODEL

Near the surface of the earth, where the momentum is transferred down through the layer to the surface, the diffusivity for momentum can be shown to be given by the following equation:

$$k_m = \frac{k\, U_* Z}{\phi\left(\frac{Z}{L}\right)} \qquad (5)$$

where the quantity in the numerator is the diffusivity for neutral conditions ($z/_L = 0$) and the quantity $\phi\left(\frac{Z}{L}\right)$ is a function of stability called the phi-function. Various empirical and theoretical expressions exist for the "phi-function". From the work of Businger, et al(4), the phi-function can be defined as:

$$\text{stable:} \quad \phi\left(\frac{Z}{L}\right) = 1 + 4.7\left(\frac{Z}{L}\right) \qquad (6)$$

$$\text{unstable:} \quad \phi\left(\frac{Z}{L}\right) = \left[1 - 15\left(\frac{Z}{L}\right)\right]^{-0.25} \qquad (7)$$

where the coefficients were empirically determined. The following discussion will indicate the range of applicability of these functions.

The friction velocity, U_*, may be determined from the stability modified log-law given by the following equation:

$$\frac{\partial u}{\partial z} = \frac{U_*}{k_Z}\, \phi\left(\frac{Z}{L}\right) \qquad (8)$$

where U is the mean wind speed measured at height z_w. Integrating equation (8) from $z = z_o$ (where U = 0) to $z = z_w$, we obtain the following:

$$U_* = \frac{k\, U_{Zw}}{\int_{Z_O}^{Z_W} \frac{\phi\left(\frac{Z}{L}\right)\partial z}{Z}} \qquad (9)$$

where z_w = height of surface winds measured above average canopy height. The expression for z_w can be defined as

$$z_w = z_u - h_c$$

where z_u = height above ground surface where wind speeds are measured
h_c = average height of canopy.

Figure 7 illustrates the relationships between h_c, Z_w, and Z_u.

We have taken U_* as constant with height (constant flux layer assumption).

Depending on the accuracy desired, the integral in equation (9) may be integrated exactly or approximately. If the stability parameter, $|\frac{Z}{L}|$ is not greater than one, an approximate form of the phi-function can be chosen which is valid for both unstable and stable conditions. From the work of Morgan et al(13), this is $\phi = 1 + 2\left(\frac{Z}{L}\right)$. Equation (9) then becomes

Approximate, all stabilities

$$U_* = \frac{k\, U_{ZW}}{\left[\ln\left(\frac{Z_W}{Z_o}\right) + \frac{2}{L}\left(Z_W - Z_o\right)\right]} \qquad (10a)$$

If greater accuracy is warranted, exact integrals are available for the stable and unstable cases. The equation for U_* is then given by the following:

Exact, Stable

$$U_* = \frac{k\, U_{ZW}}{\left[\ln\left(\frac{Z_W}{Z_o}\right) + \frac{4.7}{L}\left(Z_W - Z_o\right)\right]} \qquad (10b)$$

Exact, Unstable

$$u_* = \frac{k\,u_{zw}}{\ln\left[\dfrac{\left(1-15\frac{Z_w}{L}\right)^{1/4}-1}{\left(1-15\frac{Z_w}{L}\right)^{1/4}+1}\right] + 2\tan^{-1}\left(1-15\frac{Z_w}{L}\right)^{1/4} - \ln\left[\dfrac{\left(1-15\frac{Z_o}{L}\right)^{1/4}-1}{\left(1-15\frac{Z_o}{L}\right)^{1/4}+1}\right] - 2\tan^{-1}\left(1-15\frac{Z_o}{L}\right)^{1/4}} \qquad (10c)$$

Equations (5), (6), (7), and (10) constitute a complete model for calculating the diffusivity near the surface of the earth. To use the model, $z/_L$ must be determined from, for instance, Pasquill categories, and z_o must be specified, according to site characteristics, and a measured wind must be available. The phi-functions that have been quoted are based on the common micrometeorological practice of specifying height, not from the ground, but from a reference height called the zero-plane displacement height. This height usually closely corresponds to the average height of the site roughness elements (trees, building, etc.), and its precise value is not critical. When surface roughness is small or when the calculation as being made at a height well away from the surface, this micro-meteorological nicety can be ignored. However, in urban areas, the height z_w will normally be comparable with the average roughness elements and therefore this height should be specified with respect to the zero-plane displacement height.

The data on which this model is based cover the stability range, $-2.5 \leq z/_L \leq 1$. On the unstable side, we may reasonably extend the model to $z/_L = -5$. However, the quantity $|L|$ can be as small as 10 m and hence a different approach is needed for $-z/_L > 5$. Above this height we will use the following equation to calculate diffusivity:

$$K = C\,\epsilon^{1/3} Z^{4/3} \qquad (11)$$

where ϵ is the dissipation rate (the rate at which turbulent kinetic energy is converted to heat) and c has the value of about 0.5. This relationship goes back to the work of Richardson(14) who first noted that atmospheric diffusivities over a very wide range of scales appeared to follow a "4/3 law". The inclusion of 1/3 is made on the dimensional grounds suggested by the Kolmogorov(15) theory of turbulence. This particular functional form for diffusivity has been used previously by Panofsky(16) and discussed by Batchelor(17). The utility of this approach for the practical applications we have in mind depends on (1) the confidence one may place on the value of c and (2) the availability of a method of estimating the dissipation, ϵ. Wyngaard and Cote(18) have shown that near the surface of the earth (neutral conditions), dissipation is known to equal shear production of kinetic energy and can be expressed as:

$$\epsilon = u_*^2 \frac{\partial u}{\partial z} \quad . \tag{12}$$

Substitution of this relationship into equation (11) leads to the following relation:

$$C = k^{4/3} = (0.35)^{4/3} = 0.25 \tag{13}$$

In the pure free convection regime, dissipation is constant with height. Willis and Deardorff(19) and Lenschow(20) have shown dissipation is well approximated by:

$$\frac{\epsilon Z_i}{W_*^3} = 0.4 \tag{14}$$

where z_i is the height of the inversion which caps the convective layer and w_* is a convective velocity, analogous to, and related to, U_*, given by:

$$W_* = \left(\frac{gHZ_i}{\rho C_p T}\right)^{1/3} = \frac{1}{k^{1/3}}\left(\frac{-Z_i}{L}\right)^{1/3} u_* \tag{15}$$

where $z_i/_L$ will be recognized as the overall stability of the entire convective layer. If we require both diffusivity formulae, equations (11) and (5), to be valid at the same level, as they must if the two approaches are compatible, we obtain:

$$K = C\epsilon^{1/3} Z^{4/3} = \frac{k U_* Z}{\phi\left(\frac{Z}{L}\right)} \quad . \tag{16}$$

Substituting from equations (14) and (15) we obtain:

$$C = \frac{k^{4/3}}{\left(-0.4\,\frac{Z}{L}\right)^{1/3} \phi\left(\frac{Z}{L}\right)} \tag{17}$$

Lenschow(20) has shown that the relationship expressed by equation (14) is known to be valid down to $-z/_L = 10$. It is assumed that it remains approximately true at $-z/_L = 5$ where we are extending the unstable phi-function from below. Evaluating equation (17) for $z/_L = -5$, and using the previously given formula (equation 6) for $\phi\ (z/_L)$, we obtain $c = 0.58$, a value about twice that previously obtained for very different conditions near the ground. A more detailed analysis, using the dissipation measurements of Wyngaard and Cote(18) is given in detail by Myrup and Ranzieri(3) which shows that c tends toward a constant value of 0.46 as $Z/_L$ approaches -5. For the purposes of this diffusivity model, the authors chose to adopt $c = 0.5$ for $-z/_L > 5$.

Equations (1), (13) and (14) may be combined to give:

$$K = C\left(\frac{-0.4Z}{kL}\right)^{1/3} U_* Z \tag{18}$$

which is assumed valid for the convective layer above $-z/_L = 5$.

The diffusivities given by equation (18) are quite large. For example, for $L = -100$ m, $z_o = 1$ m (an urban value), $U = 2$ meters/sec, and $z = 100$ m, we obtain: $K = 1{,}114\ m^2/min$. If L is set at -10 m (very unstable) K increases to $10{,}130\ m^2/min$ at 100 m. However, these larger values are quite consistent with the scarce estimates which are available for diffusivity under unstable conditions well away from the surface. Lettau(21) obtained a value of 600 m^2/min at 200 m for conditions of strong instability. Woskresenski and Matwejew(22) made 225 estimates of momentum diffusivity from aircraft observations in the lowest 100 meters over the Arctic Sea. Their values generally ranged from 1,200 m^2/min to 4,800 m^2/min.

In general, the observational evidence at 100 m and above is inadequate to verify more than the order of magnitude of diffusivity estimates. In particular, more information is needed as to the shape of the diffusivity profile in the upper portions of convective layers. Diffusivity cannot increase indefinitely with height, as equation (18) states, because at some point the influence of the bounding inversion layer must act to limit the value of the diffusivity.

Under these circumstances, perhaps the best evidence available comes from sophisticated numerical boundary layer models. The most advanced approach the authors are aware of is that of Mellor and Yamada(23) who present a hierarchy of models for the planetary boundary layer based on a consistent scheme for including effects of turbulence anisotropy at various levels of approximation (closure assumptions). Using the boundary and initial conditions of Clark's(24) Wangara experiment, Mellor and Yamada integrated three models and found an adequate model to describe the known properties of the planetary boundary layer. In the late afternoon, this model generates momentum diffusivities which increase with height to about $z/zi = 0.3$ where a value near 3,000 m^2/min is attained. Using the same boundary conditions, equation (18) yields a diffusivity of 3390 m^2/min indicating good correspondence between the two approaches at this height. For $z/zi > 0.3$, the diffusivity profile calculated from Mellor and Yaruada's model shows a broad maximum in the central portion of the convective layer surmounted by an abrupt decrease to zero in the lowest portion of the bounding inversion layers.

For non-photochemical air quality modeling, the surface concentration of pollutant will be insensitive to the diffusivity value in the upper portions of the convective layer. Therefore, for inert pollutants, we now add to our diffusivity model the requirement that diffusivity be constant for $z/zi > 0.3$ and go to zero at $z/zi > 1$.

In the case of photochemical pollution, however, the mixing processes in the upper half of the convective layer are important. This complication arises from the fact that some of the important reactions are relatively slow. A consequence is that polluted air arriving at a location many miles downwind from the urban source of the primary pollutants has had time both for completion of the photochemical reactions and for complete mixing throughout the convective layer. Hence, high surface values of Ozone, for instance, commonly observed downwind of a high emissions area are partly a consequence of mixing which has occurred in the upper portions of the convective layer. Use of the constant diffusivity approximation specified above would tend to overestimate this mixing. Therefore, for photochemical pollutants we specify that for $z/zi \geq 0.1$ diffusivity calculated by the methods described above should be multiplied by the function $(1.1 - z/zi)$. This simple function has the properties of rolling off smoothly from a value of unit's at $z = 0.1\ Z_i$, allowing a maximum in the diffusivity profile in the central portion of the mixed layer and retaining a relatively small value at the base of the inversion. It thus allows some mixing with inversion air and goes to zero at $z = 1.1\ Z_i$. Above this point, the diffusivity should be held at zero. The "roll off" function should be used for photochemical pollutants for neutral and unstable conditions, in conjunction with either equation (5) or (18) (whichever is appropriate) between the heights $Z = 1.1\ Z_i$ and $Z = 0.1\ Z_i$.

The above formulations are recommended for unstable stratification ($Z/L < 0$). For the stable case diffusivity should be calculated from equations (5) and (6) throughout the depth of the mixed layer. Inasmuch as there is no way to obtain the mixing depth from surface measurements alone, this quantity must be estimated from upper air measurements. This is the same procedure as for the unstable case discussed above.

In the stable case, however, it is not necessary to specify a special upper level diffusivity model and hence the diffusivity should be set to zero at the top of the mixed layer.

LIMITATION OF DIFFUSIVITY MODEL

There are three principle limitations to this model of which the authors are aware. The first, and probably most severe, is the fetch/height requirement. The functional forms used to specify the diffusivity near the surface, equations (6) and (7), are based on measurements made in a boundary layer in which an equilibrium state has been attained between flux and gradient. The maximum height at which this state has been achieved is a function of the fetch over which homogeneous surface conditions are found upwind. It is common in micrometeorology to quote a figure of 100 as the maximum value of the fetch/height ratio at which the micrometeorological flux/gradient relationships may be used. To use this diffusivity model in regional air quality models, in the absence of any viable alternate approach, the authors feel that this figure may be lowered down to 50(27 and 28). The surface diffusivity formulation is thus assumed to be strictly valid only up to heights one-fiftieth the upwind distance over which homogeneous land-use is found. In order to extend the approach to greater heights the surface conditions such as the roughness parameter must be adjusted to reflect average conditions over an upwind fetch equal to fifty times the height in question.

A second limitation of this approach is found in the stable condition. It is commonly observed that early morning surface inversions are surmounted by a deep, neutral layer capped by an elevated stable layer. Often these higher layers are left over from the atmospheric mixing processes of the day before. Obviously, vigorous mixing can be occurring in this elevated neutral layer. As given above, our diffusivity model would "turn off" the mixing near the surface and allow nothing to occur above. In many applications where the emphasis is on surface emission and their immediate dispersal, there would be no problem. However, in some cases, such as the photochemical air pollution problem, it may be important to carry on realistic diffusion calculations above a surface inversion. In that case we recommend that diffusivity in the elevated neutral layer be calculated as if the entire layer up to the boundary stable layer aloft was neutrally stratified (very large $|L|$).

Finally, the fundamental assumption in the absence of any information to the contrary, is that the diffusing properties act like momentum in so far as specification of diffusivity is concerned. It is concieveable that some pollutants such as aerosols and particulates, may behave differently. However, even in that case, correction factors for deposition could be simple functions of stability so that the general approach proposed here should still be useful. Further research is required to fully analyze this situation.

For all situations it is necessary to know the measured wind at (ideally) a height of 10 m above the zero displacement plane (or lower with proper exposure), the aerodynamic roughness length z_o, and the Monin-Obukhov length L. z_o may be estimated from land-use or equation and L may be obtained from the Pasquill stability category.

For both stable and unstable conditions, it is necessary to know the depth of the mixed layer and to calculate the friction velocity, U_*. This may be done approximately according to:

$$U_* = \frac{k\,U_{zw}}{\ln\left[\frac{Z_w}{Z_o} + \frac{2}{L}(Z_w - Z_o)\right]} \qquad \text{Equation (10a)}$$

(1) Stable surface conditions (L > 0)

$$km = K = \frac{k\,U_* Z}{\phi\left(\frac{Z}{L}\right)} \qquad \text{Equation (5)}$$

$$\phi\left(\frac{Z}{L}\right) = 1. + 4.7\,\frac{Z}{L} \qquad \text{Equation (6)}$$

Exact form for U_*:

$$U_* = \frac{k\,U_{zw}}{\left[\ln\frac{Z_w}{Z_o} + 4.7\,(Z_w - Z_o)\right]} \qquad \text{Equation (10b)}$$

These equations are taken as valid for both inert and reactive pollutants throughout the depth of the surface layer; above this depth, calculations of diffusivity should proceed in the manner discussed below.

(2) Stable surface conditions ($L > 0$) with an elevated mixed layer.

(a) For the surface layer, use the procedure recommended above.

(b) In the elevated mixed layer, assume near-neutral (slightly unstable) conditions with a large negative value of L (the authors recommend $L = -10^5$ meters). Treat the upper portions of the elevated mixed layer exactly as the upper portion of a convective layer is treated (see below).

(3) Unstable conditions ($L < 0$)

Exact form for U_*:

$$U_* = \frac{k\,U_{ZW}}{\ln\left[\frac{\left(1-15\frac{Z_W}{L}\right)^{1/4}-1}{\left(1-15\frac{Z_W}{L}\right)^{1/4}+1}\right] + 2\tan^{-1}\left(1-15\frac{Z_W}{L}\right)^{1/4} - \ln\left[\frac{\left(1-15\frac{Z_o}{L}\right)^{1/4}-1}{\left(1-15\frac{Z_o}{L}\right)^{1/4}+1}\right] - 2\tan^{-1}\left(1-15\frac{Z_o}{L}\right)^{1/4}}$$

Equation (10c)

(a) $Z \leq -5L$

$$K = k_m = \frac{k\,U_* Z}{\phi\left(\frac{Z}{L}\right)}$$ Equation (5)

$$\phi\left(\frac{Z}{L}\right) = \left(1-15\,\frac{Z}{L}\right)^{-0.25}$$ Equation (7)

(b) $Z \geq -5L$

$$K = 0.5\left(\frac{-0.4\,Z}{k\,L}\right)^{\frac{1}{3}} U_* Z$$ Equation (18)

(c) $Z > 0.3\ Zi$, inert pollutants.
K should be held constant at whatever value assigned at $Z = 0.3\ Zi$ and set to zero at $Z \geq 1.0$

(d) Photochemical pollutants, $0.1\ Zi \leq Z \leq 1.1\ Zi$.
Diffusivity calculated either by equation (5) or (18) should be multiplied by the function $(1.1 - Z/Zi)$.
Above $Z = 1.1\ Zi$, diffusivity should remain at zero.

(4) Neutral conditions

Use equation (5) with a very large value of L with appropriate sign and, as above, holding K constant above $Z = 0.3\ Zi$ for inert pollutants.

For reactive pollutants, the diffusivity value calculated by equation (5) should be multiplied by the roll-off function

$$\left(1.1 - \frac{Z}{Z_i}\right) \text{ for } \frac{Z}{Z_i} \geq 0.1 \quad .$$

Air quality models are generally based on the solution of the species-conservation-of mass equation. This equation for a given air pollutant species and chemical reaction can be expressed as(25):

$$\frac{\partial C_i}{\partial \tau} + \frac{u \partial C_i}{\partial x} + \frac{v \partial C_i}{\theta y} + \frac{w \partial C_i}{\partial z} = \frac{\partial}{\partial x}\left[K_x \frac{\partial C_i}{\partial x}\right] + \frac{\partial}{\partial y}\left[K_y \frac{\partial C_i}{\partial y}\right] + \frac{\partial}{\partial z}\left[K_z \frac{\partial C_i}{\partial z}\right] + R_i + S_i \qquad (18)$$

where C_i = concentration of pollutant species i

x,y,z = Cartesian coordinates

u,v,w = wind speed in the x,y, and z directions respectively

K_x, K_y, K_z = horizontal and vertical turbulent diffusivities

R_i = rate of production of species i through chemical reaction

S_i = rate of production of species i from source emissions.

In this equation K_z is synonymous with K_m, the momentum diffusivity.

The numerical solution of equation (18) is solved using either an eulerian or lagrangrian coordinate system. The eulerian coordinate system is fixed to the surface of the earth while the lagrangrian coordinate system is a moving system. The eulerian solution is commonly referred to as a grid model while the lagrangian solution is a trajectory model.*

In the grid model the study region is divided into a three dimensional array of cells. Each cell can vary from 1 km to 4 km on a side and on the order of 10 to 100 meters high. The size of each cell, of course, will depend on the size of the study area, spatial distributions of emission fluxes of pollutants,

*There are versions of grid and trajectory models in the public domain that solve equation 18. The discussion that follows applies to the concept and does not necessarily endorse a specific grid or trajectory model.

and terrain affects that may alter the surface winds. The solution of equation (18) is achieved by numerically integrating the equation in three dimensional space and in time over each grid square.

In the trajectory model, a column of air is followed through the study area as it is moved by the surface winds. The pollutants are emitted into the column as fluxes at the ground surface. As the column passes over the study area chemical reactions take place in the column. The trajectory solution involves the integration of equation (18) along the trajectory path with the following assumption that $V = w = K_x = K_y = 0$. This is required in order to maintain the group of cells in the column.

Figure 8 shows a typical study area for the Los Angeles region using 3.2 x 3.2 km grid squares.

Both of these models require K_z as an imput parameter. The following discussion will illustrate how the diffusivity model presented in this report can be interfaced with the solution of equation 18.

For the given study area the wind flow field will be constructed for each grid square for each hour of simulation based on existing meteorological data. In order to use the diffusivity model presented in this report, the aerodynamic roughness parameter Zo must be estimated for each grid square. This can be done by using aerial photographs, land use plans or field inspection. Table 1, or the expression $Zo = 0.15\ h_c$, can be used as previously discussed. Once this is completed and with Z_o and $\overline{U}$ (surface winds) known, the procedure for calculating the diffusivity profiles as a function of time and location can begin.

This procedure can be followed using either a grid or trajectory model.

Grid Models (Regional)

1. For grid models, develop the hourly surface wind flow field for each grid square in the study area.

2. For each grid square (using the wind speed calculated in Step 1 above), calculate the Turner stability class using the cloud cover and ceiling height representative for each square.

In those study areas where two or more meteorological sources exist which measure cloud cover and ceiling height, care and judgment must be exercised in determining which measurement of cloud cover and ceiling height is representative of which portion of the study region. A typical example is the Los Angeles Basin where the low stratus exists along the coast but does not generally penetrate into the San Fernando Valley. Figure 9 illustrates the region and terrain in the area.

Under these conditions, the measured cloud cover and ceiling height at Burbank Airport would be most representative of the San Fernando Valley while Los Angeles International Airport is most representative for the portion of the basin along the coast.

3. For each grid, square the aerodynamic roughness height Z_o must be characterized based on Table 1 or calculated by $Z_o = 0.15\ h_c$. The Z_o should be representative of the land use in each square. This information can be obtained from aerial photographs or from a field survey.

4. The spatial and temporal distribution of surface based and elevated inversions must be described for the study area. This

may be different for portions of the study area due to the terrain effects. Care and judgment must be exercised in choosing representative inversion conditions for the study area.

5. For each three-dimensional surface and the vertical grid, the diffusivity profiles can be calculated using the diffusivity model described in this report.

6. It is suggested that the diffusivity profiles be a part of the air quality preparation program such as is done in the SAI(25) model for meteorology, emissions and initial concentrations. This would allow the user the ability to examine the diffusivity profiles before simulation runs are made.

Trajectory Models (Regional)

Figure 10 illustrates a trajectory passing over a grid for given meteorological conditions within the Los Angeles Area. Under these conditions it is necessary only to determine Z_o for those grid squares over which the trajectory passes.

The same procedures described above would apply for each such grid square.

The authors, therefore, conclude that the latest state-of-the-art diffusivity profile model can be integrated into air quality models and should provide a sound and rational approach for calculations of vertical diffusivities.

By using this diffusivity model with air quality models, a more accurate prediction of air quality can be made. This will allow transportation planners and engineers to make further refinements in evaluating the interrelationships of land use, transportation and air quality.

EXAMPLES OF DIFFUSIVITY CALCULATIONS

As an illustration of the applications of this diffusivity model, seven examples for various stabilities, land uses, and wind speeds are presented. Examples are given for diffusivities that can be used in either grid or trajectory regional air quality models. The first six examples are for inert pollutants and use the approximate solutions to calculate U_*. The last example is for reactive pollutants and uses the exact solution for U_*.

EXAMPLE 1: OFFICE BUILDING LAND-USE AND UNSTABLE CONDITIONS (INERT POLLUTANT)

Given: Figure 8 illustrates the study area and the grid to be used to be used to preduct air quality. Let us assume for the sake of simplicity that the particular grid square of interest is representative of an office building district with low evaporation rate. The average height of the canopy within the grid square is 11.7 meters (38 feet). This is estimated from land use plans and zoning restrictions. Each grid square has surface dimensions of 2 km x 2 km on a side (typical for study areas of this size).

The base height of the afternoon elevated inversion is 500 m. Assume that for the grid square of interest the surface wind flow field, or trajectories, were computed by algorithms in such models as SAI Airshed Model(25) or general Research Corporation Difkin Model(26). Let us further assume that the constructed surface wind field and trajectores were based on the wind system exposure criteria recommended by Beaton, et al(6) at 10 m above the canopy or the average roughness elements. Therefore, the surface wind flow field and trajectories are valid for the area.

For the grid square of interest (grid A) the wind speed was calculated to be 4 m/sec for a midday condition. The cloud cover and ceiling height information were obtained from the closest airport and were assumed representative of the grid square in question. Based on the calculated wind speed, cloud cover, and ceiling height, Turner's Stability Class C was calculated for the base height.

Find: Vertical turbulent diffusivity for heights of 25 m up to the inversion.

Solution:

1. Calculate Z_o using equation (4).

$$Z_o = 0.15\ h_c = 0.15\ (11.7) = 1.75\ m$$

2. For this case with Stability Class C, Z_o = 1.75 m, and low evaporation (Table 3) obtain 1/L ~ 0.004.

Therefore L = -1/0.004 = -250 m

3. Calculate U_* using equation (10a)

$$U_* = \frac{k U_{zw}}{\ln\left(\frac{Z_w}{Z_o}\right) + \frac{2}{L}(Z_w - Z_o)}$$

Where Zw = 10 meters, Zo = 1.75 m, L = -250 m, k = 0.35.

Therefore, $U_* = \dfrac{0.35\ (4)}{\ln\left(\frac{10}{1.75}\right) - \frac{-2}{250}(10 - 1.75)} = 0.83$ m/sec

4. For Z = 25 m calculate the phi-function from equation (7)

$$\phi\left(\frac{Z}{L}\right) = \left(1 - 15\frac{Z}{L}\right)^{-0.25}$$

$$\phi\left(\frac{Z}{L}\right) = \left(1 - 15\frac{25}{-250}\right)^{-0.25} = 0.793$$

5. For Z ≤ -5 where Z = 25 m

$$K = \frac{k U_* Z}{\phi\left(\frac{Z}{L}\right)} = \frac{0.35\ (0.83)(25)}{0.793} = 9.2\ m^2/sec$$

OR

$$K = 9.2\ m^2/sec \times 60\ sec/min = 551\ m^2/min$$

Similar calculations can be made for various vertical heights, Z, as shown in the following table. For this example, $-\frac{Z}{L}$ never exceeds 5 so that the upper level model (equation 18) was not needed. Above 150 m the diffusivity remains constant as $\frac{Z}{Z_i} = \frac{150}{500} = 0.3$

is reached at that height.

Z (m)	Z/L	Z/Zi	$K(m^2/min)$
25	-0.10	0.05	551
50	-0.20	0.10	1240
75	-0.30	0.15	2014
100	-0.40	0.20	2852
150	-0.60	0.30	4676
200	-0.80	0.40	4676
300	-1.20	0.60	4676
400	-1.60	0.80	4676
500	-2.00	1.00	4676
600	-----	-----	0

EXAMPLE 2: LIGHT DENSITY RESIDENTIAL AREA AND UNSTABLE CONDITIONS (INERT POLLUTANT)

Given: Same conditions as in Example 1 except that the Turner Stability Class is B, wind speed at 10 m above canopy is 2 m/sec and elevated inversion 1000 m. The site is located in a light-density residential area with a moderate evaporation rate and average canopy height of 7.2 m (24 feet).

Find: Vertical diffusivity for heights above 25 m up to the inversion.

Solution:

1. Calculate Z_o using equation (4)

$$Z_o = 0.15\, h_c = 0.15\,(7.2) = 1.08 \text{ m}$$

2. For this grid with Stability Class B, Z_o = 1.08 m and moderate evaporation (Table 3), obtain

$$\frac{1}{L} \sim -0.035$$

$$\text{Therefore} \quad L \sim \frac{1}{.035} = -29 \text{ m}$$

3. Calculate U_* using equation (10a) with Z_w = 10 m, Z_o = 1.08 m, k = 0.35 and U = 2 m/sec.

$$U_* = \frac{0.35\,(2)}{\ln\left(\frac{10}{1.08}\right) - \frac{2}{29}\,(10 - 1.08)} = 0.43 \text{ m/sec}$$

4. For Z = 25 m calculate phi-function equation (7)

$$\phi\left(\frac{Z}{L}\right) = \left[1 - 15\left(\frac{25}{-29}\right)\right]^{-0.25} = 0.518$$

5. For $Z \leq -5$ where Z = 25 m

$$K = \frac{k\,U_* Z}{\phi\left(\frac{Z}{L}\right)} = \frac{0.35\,(0.43)\,(25)}{0.518} = 7.26 \text{ m}^2/\text{sec}$$

OR

$$K = 7.26 \text{m}^2/\text{sec} \times 60 = 441 \text{ m}^2/\text{min}$$

EXAMPLE 3: CENTRAL BUSINESS DISTRICT AND NEUTRAL CONDITIONS (INERT POLLUTANTS)

Given: Same conditions as in Example 1 except that the Turner Stability Class is D, wind speed is 5 m/sec at 10 m above the canopy. The site is located in the central business district with a low evaporation rate and average canopy height of 21.4 m (70 feet). The elevated inversion is at 500 m.

Find: Vertical diffusivity from 25 m up to the inversion.

Solution:

1. Calculate Zo using equation (4)

$$Zo = 0.15\ (21.4) = 3.21\ \text{m}$$

2. For the neutral case it is recommended that equation (6) be used for the phi-function with L equal to 10^5 m. The diffusivity above $Z/Z_i = 0.3$ remains constant until the inversion is reached.

3. Calculate U_* using equation (10a) with $Z_W = 10$ m, Zo = 3.21 m, k = 0.35, L = 10^5 m, $\overline{U} = 5$ m/sec

$$U_* = \frac{0.35\ (5)}{\ln\left(\frac{10}{3.21}\right) + \frac{2}{10^5}\ (10 - 3.21)} = 1.54\ \text{m/sec}$$

4. Calculate the phi-function using equation (6)

$$\phi\left(\frac{Z}{L}\right) = 1 + 4.7\left(\frac{Z}{L}\right)$$

However, since L is a large number 10^5 m, $\phi\left(\frac{Z}{L}\right)$ approaches 1.0. Therefore, $\phi\left(\frac{Z}{L}\right)$ for all practical purposes of Z's up to the inversion is equal to 1.0.

5. Calculate K using equation (5)

$$K = \frac{k\ U_* Z}{\phi\left(\frac{Z}{L}\right)}$$

Where ϕ (Z/L) = 1.0 for the neutral case

a. Sample calculations for K at Z = 25 m

$$K = 0.35\ (1.54)\ 25 = 13.5\ m^2/sec$$
$$K = 13.5 \times 60\ sec/min = 807\ m^2/min$$

6. Similar calculation can be made for various vertical heights, Z, as shown in the following table:

Z (m)	Z/Zi	K(m^2/min)
25	0.05	807
50	0.10	1613
75	0.15	2417
100	0.20	3219
150	0.30	4817
200	0.40	4817
400	0.80	4817
500	1.00	4817
600	----	----

6. Similar calculations can be made for various vertical heights, Z, as shown in the following table. The upper level diffusivities, calculated with equation (18) are shown in parenthesis for values below -Z/L = 5 so that agreement with the low level in the region of overlap may be judged. The diffusivity remains constant as Z/Zi = 0.3 is reached.

Z (m)	Z/L	Z/Zi	Eq. 5 K(m^2/min)	Eq. 18 K(m^2/min)
25	-0.86	0.025	441	
50	-1.72	0.05	1039	
100	-3.45	0.10	2460	(2038)
200	-6.90	0.20	5836	(5134)
300	-10.34	0.30		(8815)
400	-13.79	0.40		"
600	-20.69	0.60		"
800	-27.59	0.80		"
1000	-34.48	1.00		"
1200	-----	-----	-----	-----

a) Sample calculation of K for upper level diffusivity equation (18).

$$K = 0.5 \left(-\frac{0.4Z}{kL}\right)^{\frac{1}{3}} U_* Z$$

For $Z = 300$ m $(Z \geq -5L)$, $k = 0.35$, $L = -29$ m,

$U_* = 0.43$ m/sec.

$$K = 0.5 \left[\frac{-0.4\,(300)}{0.35\,(-29)}\right]^{\frac{1}{3}} (0.43)\,300 = 147 \text{ m}^2/\text{sec}$$

or

$$K = 147 \text{ m}^2/\text{sec} \times 60 = 8816 \text{ m}^2/\text{min.}$$

EXAMPLE 4: RURAL AREA WITH NEUTRAL CONDITIONS (INERT POLLUTANT)

Given: Same conditions as Example 3 except that the site is located in a seasonal green agricultural area with a high evaporation rate.

Find: Vertical diffusivities from 25m to inversion.

Solution:

1. From Table 1 assume Zo = 0.0272 m (alfalfa)

2. Calculate U_* using equation (10a) and $L = 10^5$

$$U_* = \frac{0.35\,(5)}{\ln\left(\frac{10}{0.0272}\right) + \frac{2}{10^5}\,(10-0.0272)} = 0.0487 \text{ m/sec}$$

3. Calculate the phi-function. As previously discussed in Example 3, ø (Z/L) is equal to 1.0 for neutral case.

4. Calculate K using equation (5) with ø (Z/L) = 1.0

$$K = k\,U_*\,Z$$

a. Sample calculation for Z = 25 m.

$K = 0.35\ (0.0487)\ 25 = 0.426\ m^2/sec$
$K = 0.426\ m^2/sec \times 60 = 25\ m^2/min$

Similar values of K for various heights of Z's are shown in the following table:

Z (m)	Z/Zi	K(m^2/min)
25	0.05	25.6
50	0.10	51.3
75	0.15	76.6
100	0.20	102.5
150	0.30	153.5
200	0.40	153.5
400	0.80	153.5
500	1.00	153.5
600	----	-----

The reader should note the order of magnitude difference in the vertical diffusivity over a grassy area compared to urban area (Example 3).

EXAMPLE 5: LIGHT-DENSITY RESIDENTIAL AREA WITH WIND STATION IMPROPERLY EXPOSED (INERT POLLUTANT)

Given: Same conditions as Example 2 (Light Residential Area) with moderate evaporation rate) except the height of the wind station used to construct the wind flow field or trajectories is improperly exposed. This is typical of many of the existing sources of data from local air pollution control districts. Assume average canopy height (hc) is 7.2 m and the height above ground surface of measured wind speed is 10 m.

Find: The effects of improper exposure on vertical diffusivities from 25 m to the base of the inversion.

Solution:

1. Zo = 1.08 m previously calculated in Example 2.

2. L = -29 from Example 2.

3. Calculate U_* using equation (10a) with U = 2m/sec, Zo = 1.08 m, h = 0.35, L = -29m and Zw = 10 - 7.2 = 2.8 m.

$$u_* = \frac{0.35\,(2)}{\ln\left(\frac{2.8}{1.08}\right) - \frac{2}{29}\ (2.80 - 1.08)} = 0.747 \text{ m/sec}$$

4. Calculate phi-function equation (7) for Z = 25 m.

$$\phi\left(\frac{Z}{L}\right) = 0.518 \quad (\text{Same as Example 2})$$

5. For $Z \leq -5L$ where Z = 25 m

$$K = \frac{k u_* Z}{\phi\left(\frac{Z}{L}\right)} = \frac{0.35\,(0.747)\,25}{0.518} = 12.6 \text{ m}^2/\text{min}$$

or

$$K = 12.6 \text{ m}^2/\text{sec} \times 60 = 757 \text{ m}^2/\text{min}$$

6. Similar calculations can be made for various Z heights as shown in the following table.

Z(m)	Z/L	Z/Zi	Example 2 K(m^2/min)	Example 5 Km^2/min
25	-0.86	0.025	441	757
50	-1.72	0.05	1039	1810
100	-3.45	0.10	2460 (2218)	(4280 (3860)
200	-6.90	0.20	5836 (5587)	(10150)(9700)
300	-10.34	0.30	9591	16650
400	-13.79	0.40	9591	16650
600	-20.69	0.60	9591	16650
800	-27.59	0.80	9591	16650
1000	-34.48	1.00	9591	16650
1200	- - -	- -	- -	- - -

Since U_* is the only variable that changes in calculating K, the percent change in diffusivity assuming proper exposure of Example 2 as baseline is:

$$\% \text{ Change in K} = \left[\frac{U_{*2} - U_{*5}}{U_{*2}}\right] \times 100\%$$

where $U_{*2} = 0.43$ m/sec and $U_{*5} = 0.747$ m/sec.

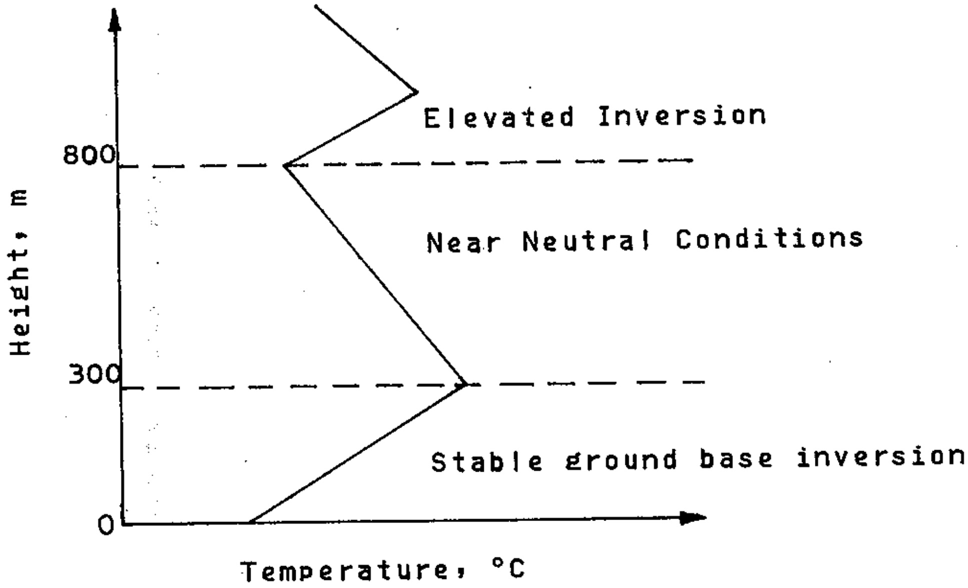
Therefore, % change is

$$\% = \left[\frac{0.430 - 0.747}{0.430}\right] \times 100 = 74\%$$

This calculation emphasizes the importance of having proper exposure of meteorological wind stations to describe the surface wind fields and trajectories when applying regional air quality models. This also stresses that the diffusivities are not free parameters in models which may be adjusted to make model predictions agree with measured data.

EXAMPLE NO. 6: LIGHT-DENSITY RESIDENTIAL URBAN AREA WITH STABLE SURFACE CONDITIONS WITH ELEVATED INVERSION (INERT POLLUTANT)

Given: Assume that for the light-density residential area of moderate evaporation rate, the calculated Turner Stability Category is F. The wind speed is measured 10 m above the canopy and is 1 m/sec. The average height of the canopy is 7.2 m (24 feet). The vertical temperature profile is shown below, with the base of the elevated inversion at 800 m.



Find: Vertical turbulent diffusivities for heights of 50 m to the base of the elevated inversion.

Solution:

1. Calculate Zo using equation (4).

$$Zo = 0.15\ h_c = 0.15\ (7.2) = 1.08\ m.$$

2. For this site with Stability Class F, the stability class must be moved one category toward the unstable condition to allow for the urban heat island effect. In this case F category becomes E. Stability Class E is now used to obtain values of 1/L. Therefore, with Stability Class E, Zo = 1.08m and moderate evaporation rate (Table 3) and using Figure 6, obtain $1/L \sim 0.005$.

Therefore, $L \sim \frac{1}{0.005} = 200\ \text{m}$

3. Calculate U_* using equation (10a)

$$U_* = \frac{0.35\ (1)}{\ln\left(\frac{10}{1.08}\right) + \frac{2}{200}\ (10 - 1.08)} = 0.16\ \text{m/sec.}$$

4. For Z = 50 m calculate the phi-function using equation (6).

$$\phi\left(\frac{Z}{L}\right) = 1 + 4.7\left(\frac{Z}{L}\right) = 1 + 4.7\left(\frac{50}{200}\right) = 2.18$$

5. Calculate the diffusivity for the surface conditions up to 300 m using equation (5).

$$K = \frac{k\, U_*\, Z}{\phi\left(\frac{Z}{L}\right)}$$

Where $k = 0.35$, $U_* = 0.16$ m/sec, $Z = 50$ m, and $\phi\left(\frac{Z}{L}\right) = 2.18$. Therefore,

$$K = \frac{0.35\ (0.16)\ 50}{2.18} = 1.28\ \text{m}^2/\text{sec} = 77.06\ \text{m}^2/\text{min.}$$

6. Similar calculations can be made for various vertical heights, Z, as shown in the following table for the surface up to 300 m.

Z(m)	Z/L	ø(Z/L)	K(m^2/min)
50	0.25	2.18	77
100	0.50	3.35	100
150	0.75	4.53	111
200	1.00	5.70	117
250	1.25	6.88	122
300	1.50	8.05	125

7. Calculate the diffusivities from 300 m to 500 m (assuming a mixed layer, near neutral conditions).

8. In this example, where $Z \leq -5L$ ($L = -10^5$ m and $Z = 350$ m), calculate ø (Z/L) using equation (7).

$$\phi\left(\frac{Z}{L}\right) = \left(1 - 15\,\frac{Z}{L}\right)^{-0.25} = \left[1 - 15\left(\frac{350}{10^5}\right)\right]^{-0.25} = 0.99$$

9. Calculate K using equation (5)

$$K = \frac{k\,U_* Z}{\phi\left(\frac{Z}{L}\right)} = \frac{0.35\,(0.16)\,(350)}{0.99} = 19.40\ m^2/\text{sec.} = 1164\ m^2/\text{min.}$$

10. Similar calculations can be made for various vertical heights, Z, as shown in the following table for 350 m to 800 m above the ground surface for $Z \leq -5L$.

Z(m)	ø(Z/L)	Z*/Zi	K(m^2/min)
350	0.99	0.10	1164
400	0.98	0.20	1371
450	0.98	0.30	1543
500	0.98	0.40	1543*
600	0.98	0.60	1543
700	0.97	0.80	1543
800	0.97	1.00	1543

*Z/Zi value for the neutral layer are base on zero datum at 300 m.

(top of stable air mass). Therefore, Z/Zi for 350 m is equal to (350-300/500 = 0.10 where 500 is the depth of the neutral layer (800 m - 300 m = 500 m).

** The diffusivities above Z/Zi = 0.30 remain constant up to the base of the inversion for the inert pollutants as shown in the above table.

EXAMPLE NO. 7: LIGHT-DENSITY RESIDENTIAL AREA WITH MODERATE EVAPORATION RATE AND UNSTABLE CONDITIONS (REACTIVE POLLUTANT)

Given: Same conditions as in example 2 except that the diffusivity is to be used with a photochemical diffusion model. As before $Zo = 1.08$ m, $L = -29$m, $U_* = 0.43$ n.sec. In this case, the calculation is made precisely as in Example 2 except that, for $Z \geq 0.1$ Zi (i.e., 100 meters), the calculated diffusivity is multiplied by the roll-off function rather than holding it constant above 0.3 Zi. Shown below are the results of this calculation in which the outputs of equation (5) (surface layer model), equation (18) (outer layer model) and the result of multiplying by the roll-off function are presented. The proper value to use in the diffusion calculation, according to the methodology presented in this report is underlined.

			Diffusivity (M^2/min)		
Z(m)	Z/L	Z/Zi	Surface Layer	Outer Layer	Roll-Off
25	-0.86	0.025	441*(416)**		
50	-1.72	0.05	1039 (981)		
100	-3.45	0.10	2460 (2322)	2038* (1924)**	2038* (1924)**
200	-6.90	0.20	5836 (5510)	5134 (4848)	4621 (4363)
300	-10.34	0.30		8815 (8323)	7052 (6659)
400	-13.79	0.40		12937	9056 (8550)
600	-20.69	0.60		22213	11107 (10487)
800	-27.59	0.80		32598	9779 (9234)
1000	-34.48	1.00		43894	4389 (4144)
1100	- - -	1.10		49841	---- ----

* Diffusivities calculated using equation 10a for friction velocity

**Diffusivities calculated using equation 10c for friction velocity.

In this example, the more exact method of calculating U_* gave a value of 0.406 m/sec. For situations closer to neutral stability, the approximate value would be more nearly equal to the exact value. Diffusivities calculated with the exact value for the friction velocity are shown in parentheses. In this case the corrected diffusivities are about 5% less. This is probably within the overall uncertainty involved in estimating diffusivity by this method and, hence, use of the corrected value is largely a matter of choice.

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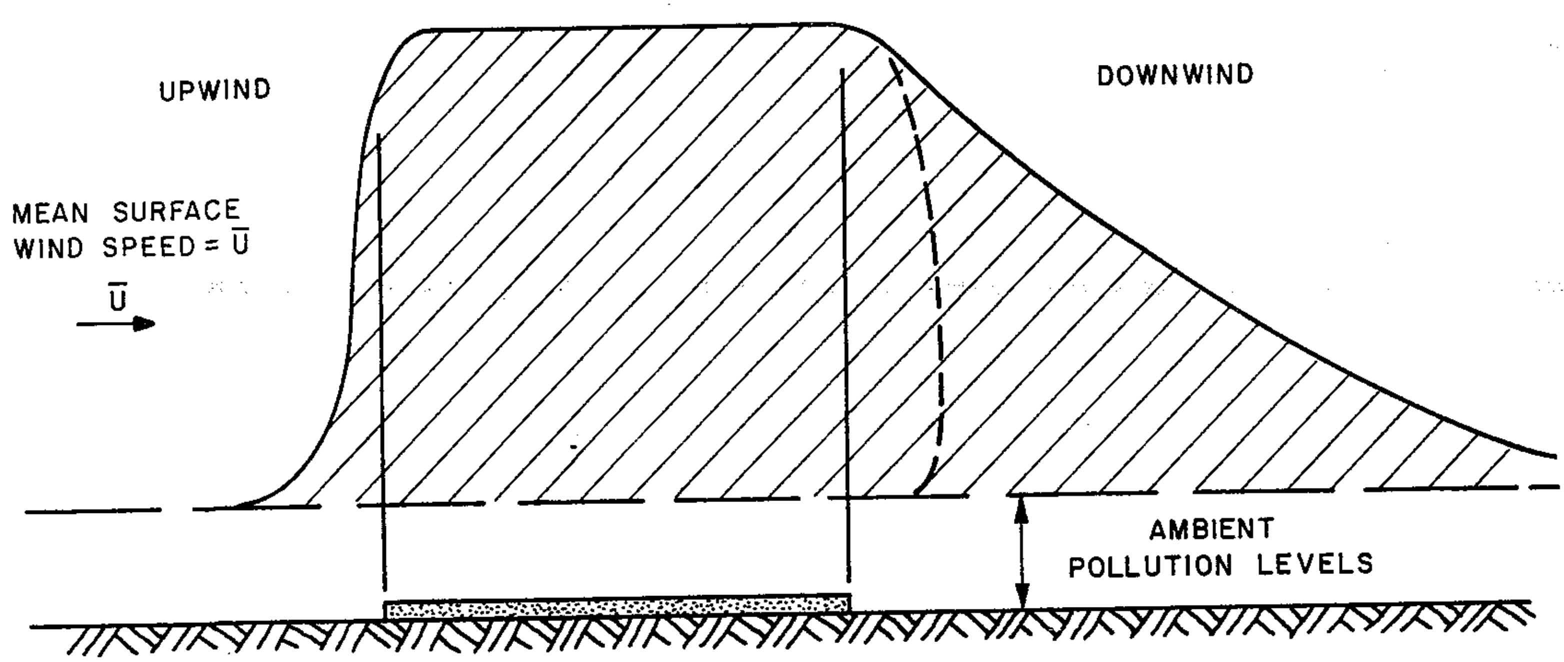

FIG. 1 MICROSCALE REGION FOR HIGHWAY IMPACT ON AIR QUALITY

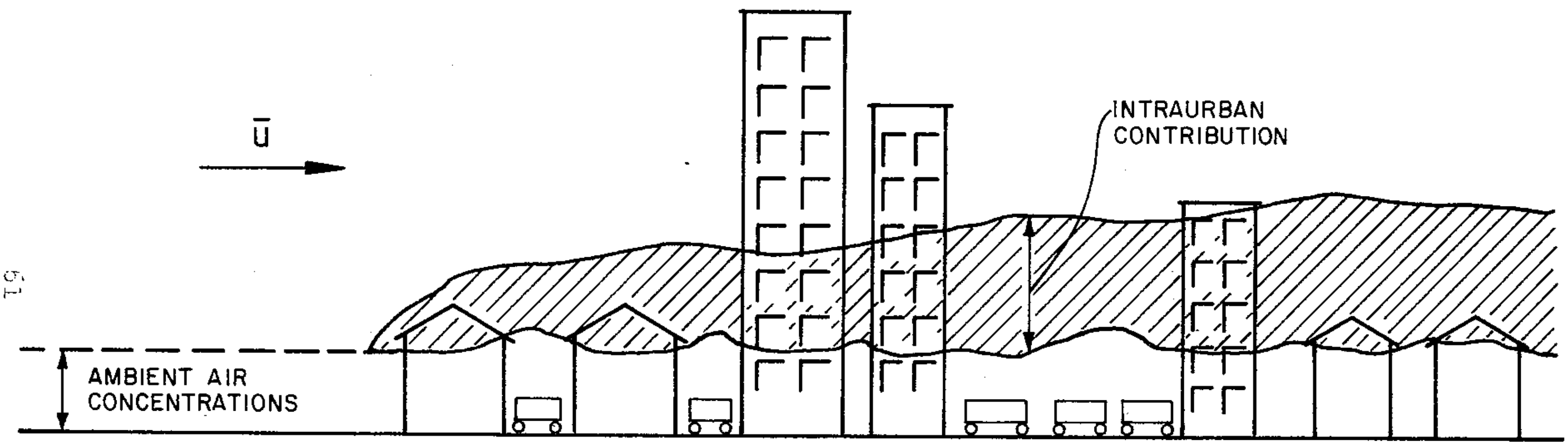

FIG. 2 MESOSCALE IMPACTS FOR AIR POLLUTION BUILD UP IN A REGION

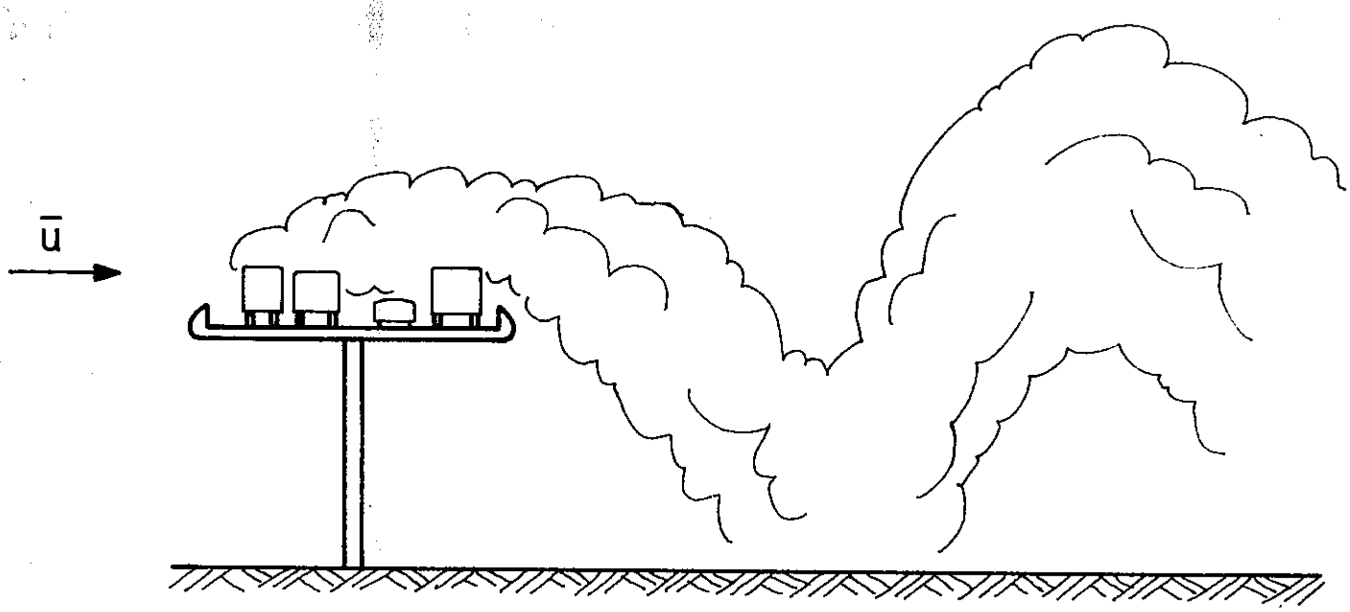

FIG. 3 DISPERSION OF POLLUTANTS EMITTED FROM A VIADUCT SECTION FOR UNSTABLE CONDITIONS

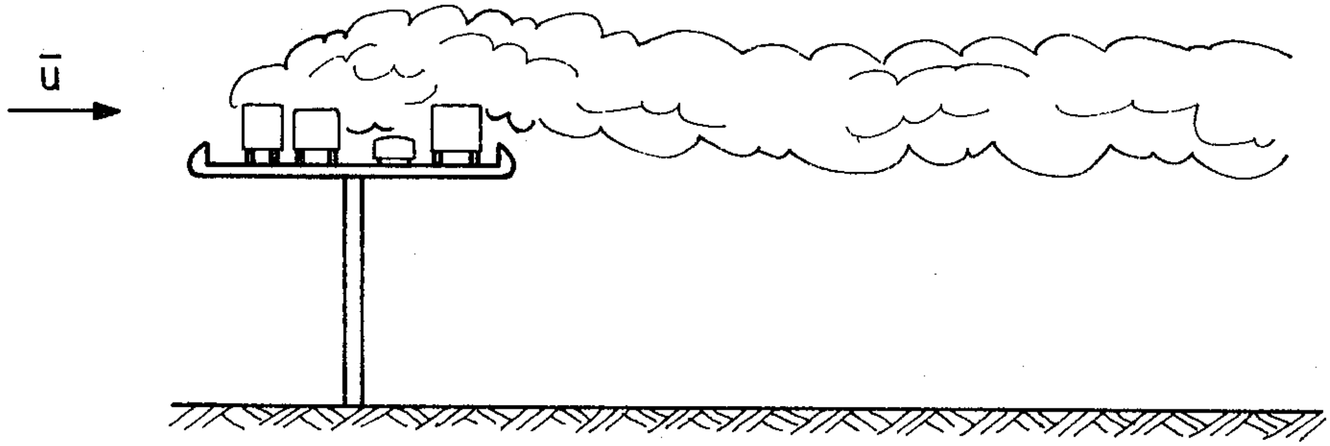

FIG. 4 DISPERSION OF POLLUTANTS EMITTED FROM A VIADUCT SECTION FOR STABLE CONDITIONS

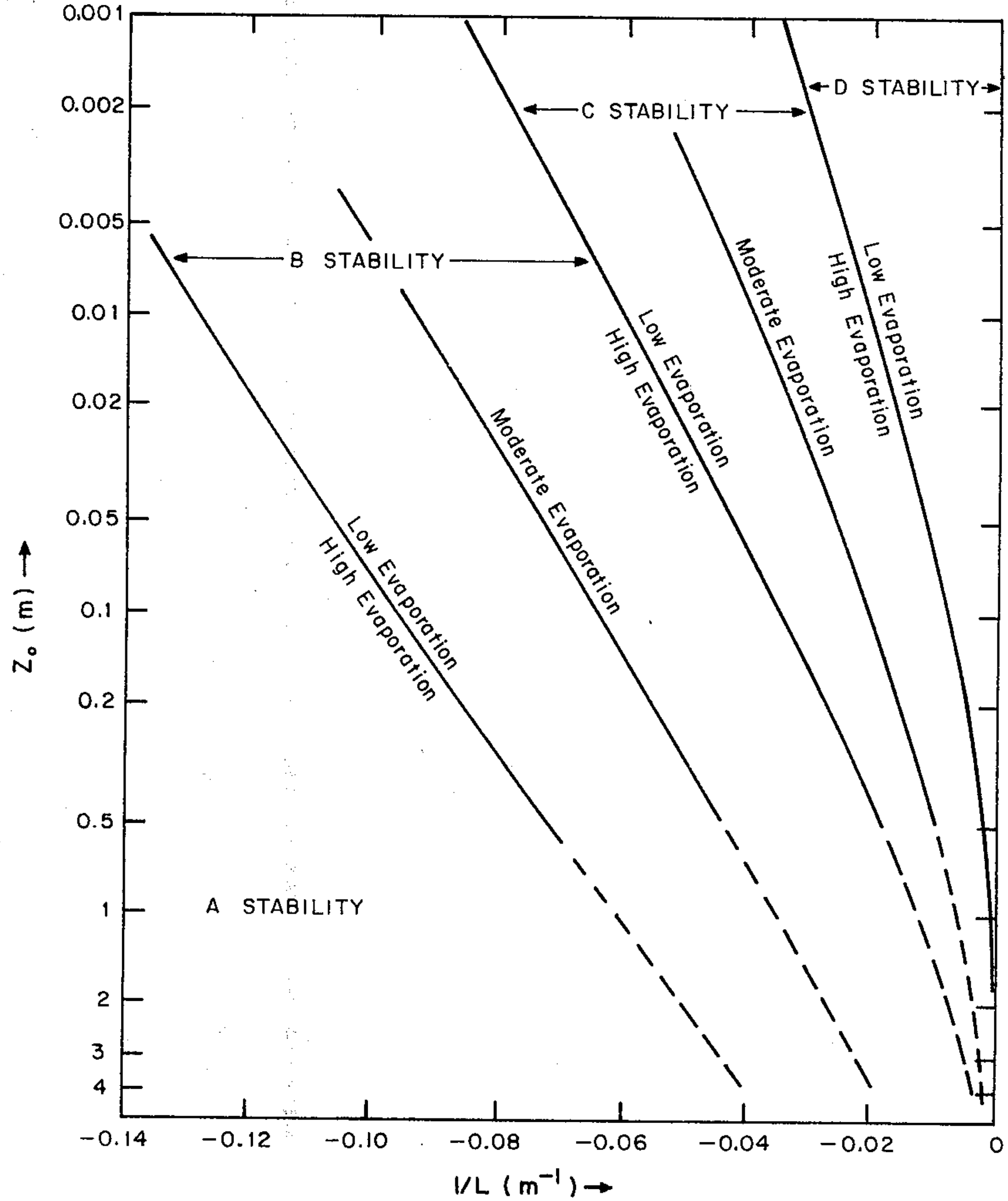

FIG. 5 I/L AS A FUNCTION OF PASQUILL STABILITY CLASSES AND Z_o FOR UNSTABLE CONDITIONS

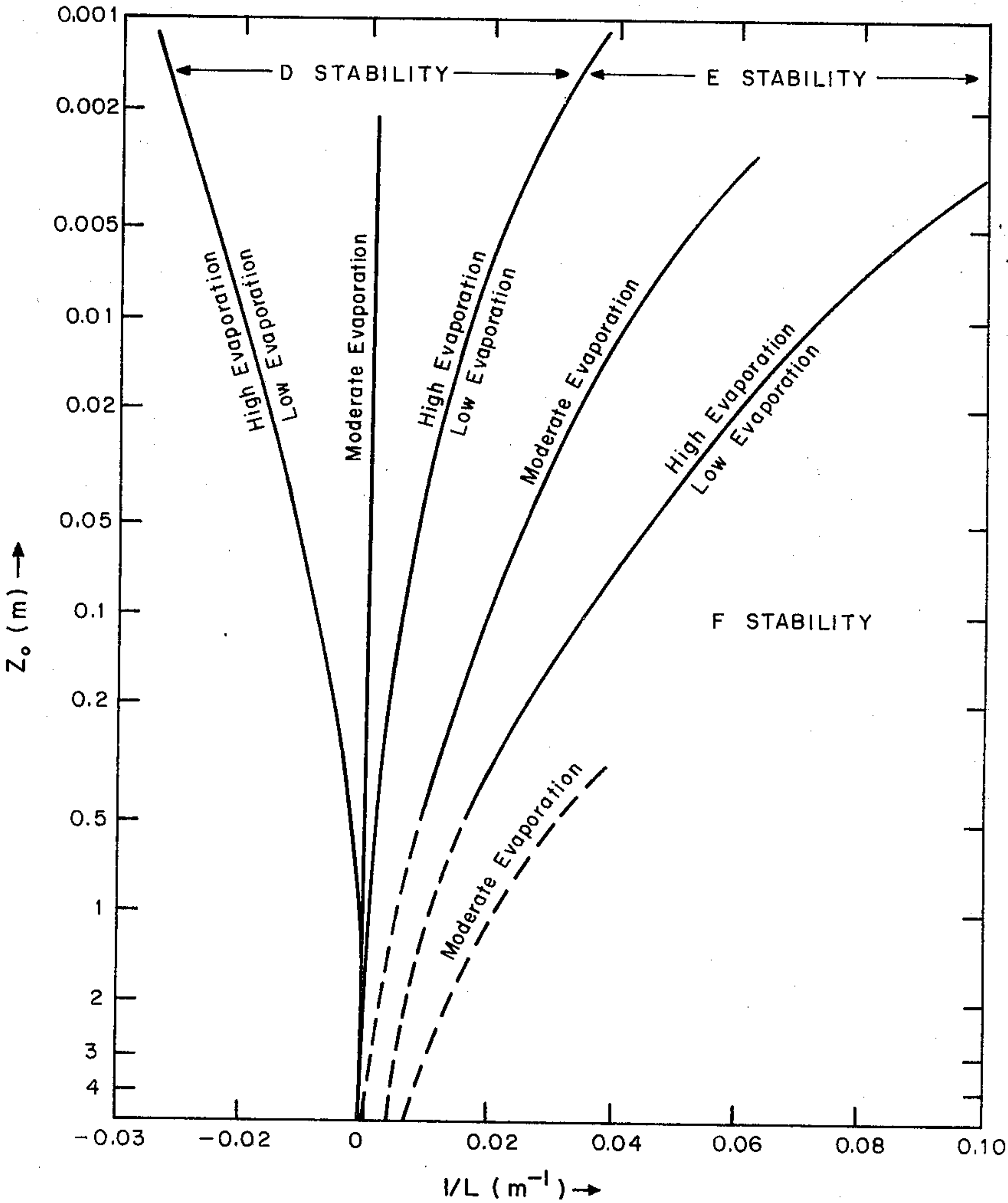

FIG. 6 1/L AS A FUNCTION OF PASQUILL STABILITY CLASSES AND Z_o FOR STABLE CONDITIONS

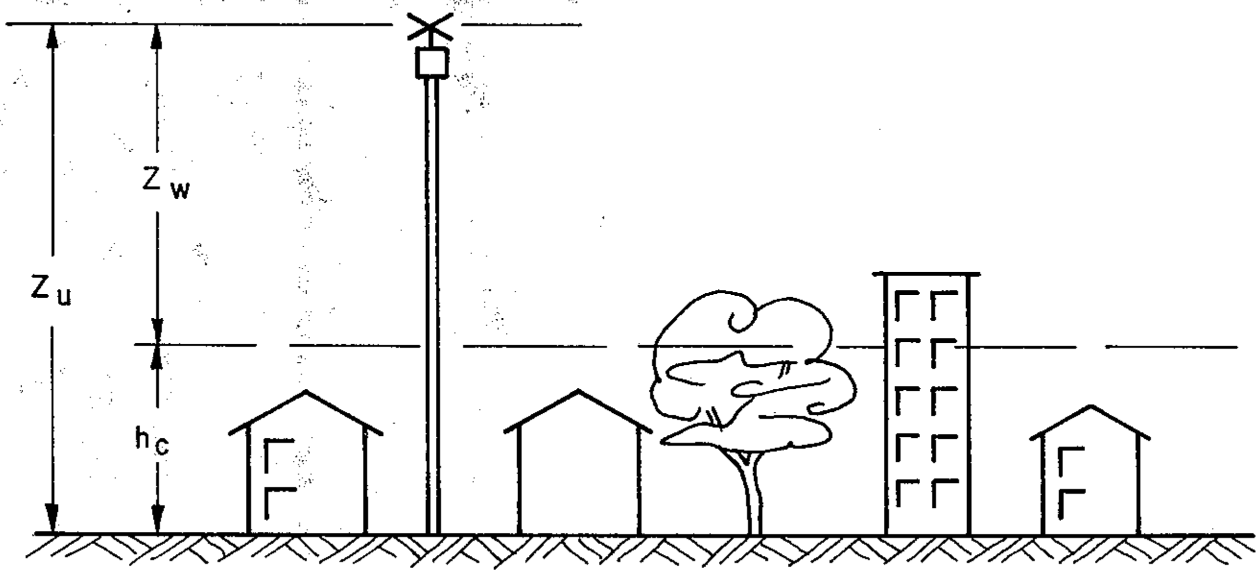

FIG. 7 RELATIONSHIP OF h_c, Z_w, AND Z_u

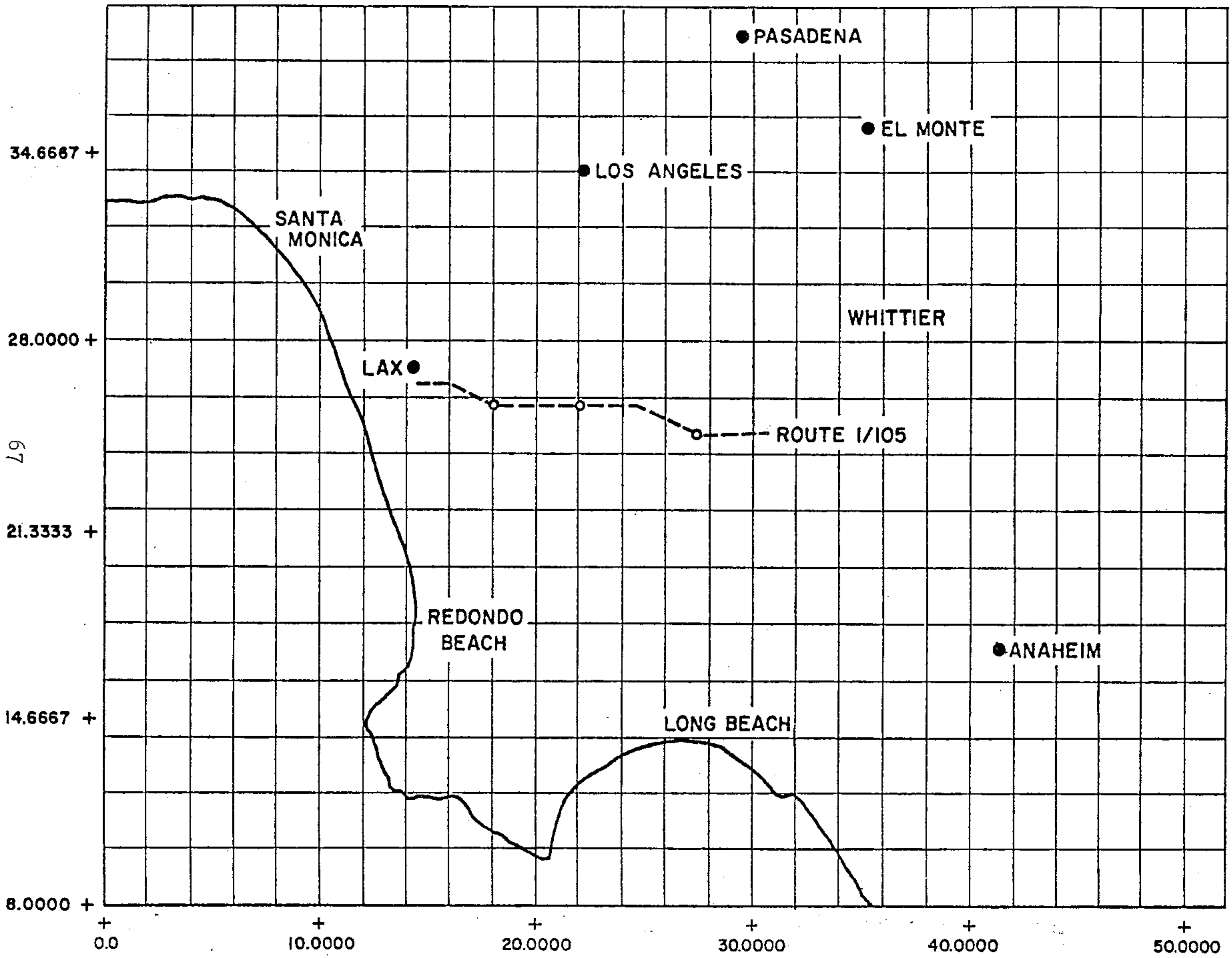

FIG. 8 TYPICAL GRID STUDY AREA FOR LOS ANGELES

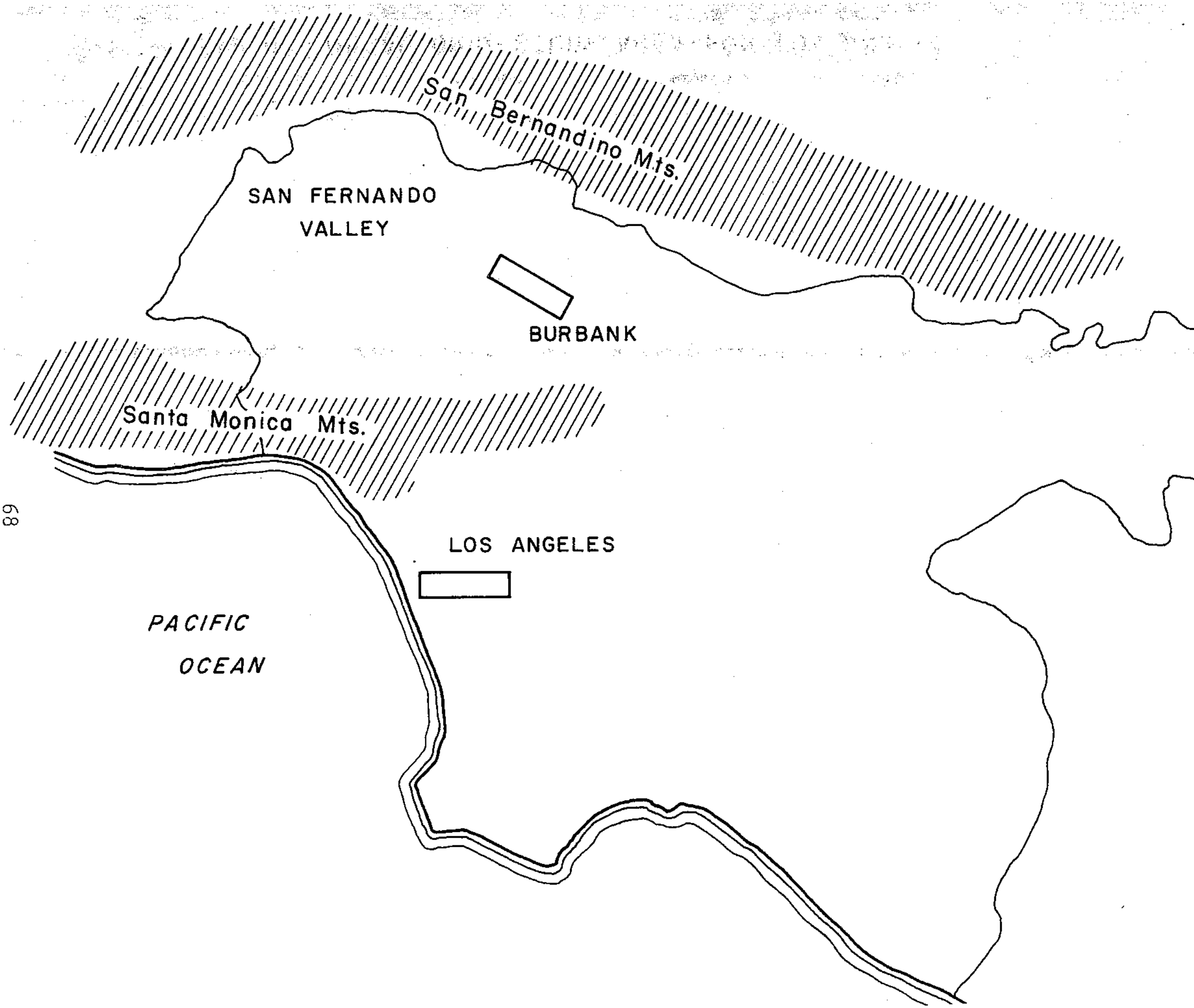

FIG. 9 ESTIMATING SURFACE STABILITY FROM TWO OR MORE AIRPORTS

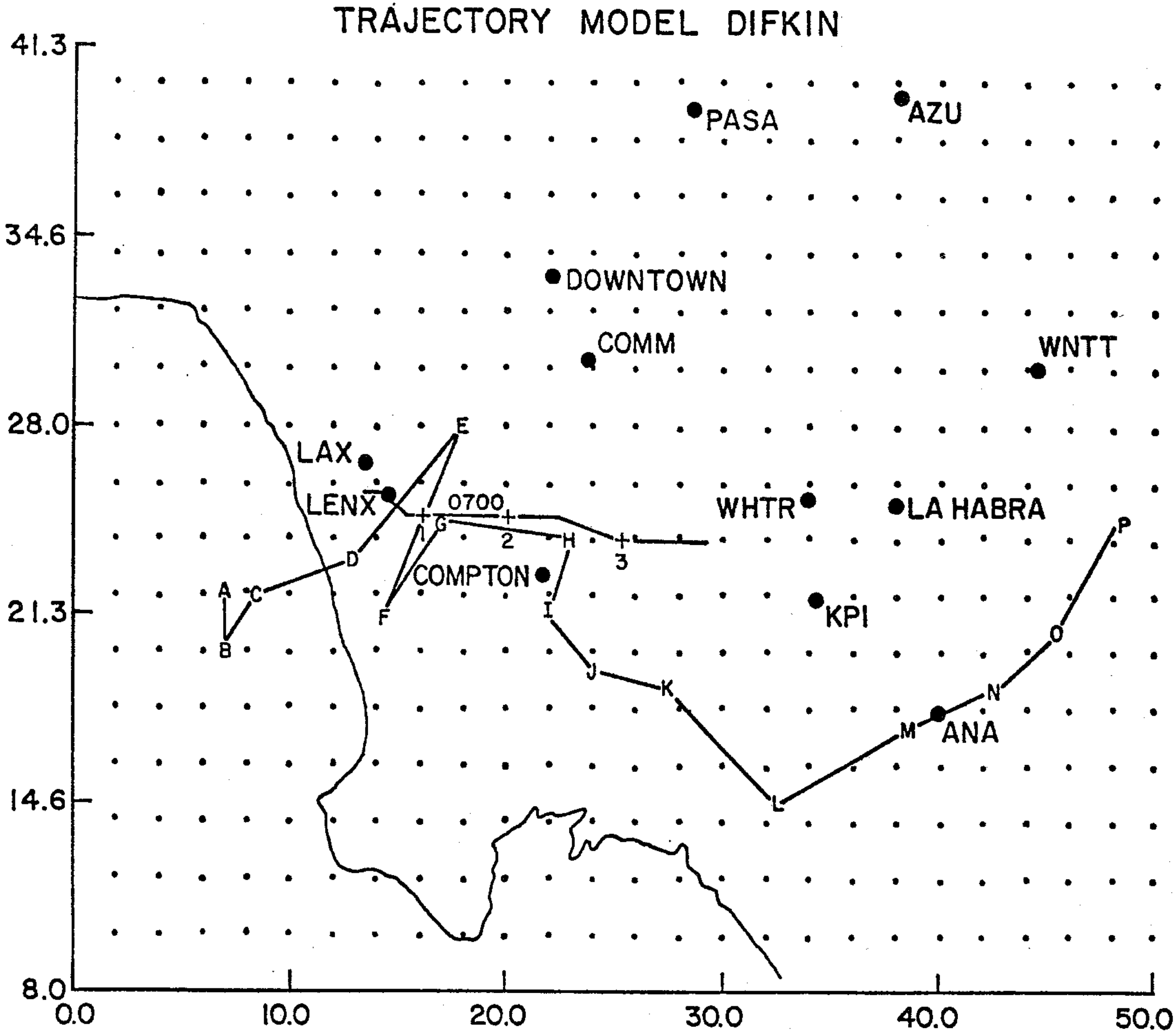

FIG. 10 TYPICAL AIR TRAJECTORY SIMULATION FOR LOS ANGELES AREA